

WEST Search History

DATE: Monday, September 22, 2003

<u>Set Name</u> side by side	<u>Query</u>	<u>Hit Count</u>	<u>Set Name</u> result set
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DB=USPT,PGPB,JPAB,EPAB,DWPI; PLUR=YES; OP=OR

L8	L7 not 2001	9	L8
L7	L6 and synthesis	174	L7
L6	L5 and variant	177	L6
L5	L4 and scaffold	180	L5
L4	L3 and secondary adj6 library	1380	L4
L3	primary adj4 library	2188	L3
L2	primar adj4 library	0	L2

DB=USPT; PLUR=YES; OP=OR

L1	5510240.pn.	1	L1
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END OF SEARCH HISTORY

Prediction of protein secondary structure using the 3D-1D compatibility algorithm

AU Ito, Masahiro; Matsuo, Yo; Nishikawa, Ken

SO CABIOS, Computer Applications in the Biosciences (1997), 13(4), 415-423
CODEN: COABER; ISSN: 0266-7061

PY 1997

AB A new method for the prediction of protein secondary structure is proposed, which relies totally on the global aspect of a protein. The prediction scheme is as follows. A structural **library** is first scanned with a query sequence by the 3D-1D compatibility method developed before. All the structures examd. are sorted with the compatibility score and the top 50 in the list are picked out. Then, all the known **secondary** structures of the 50 **proteins** are globally aligned against the query sequence, according to the 3D-1D alignments. Prediction of either .alpha. helix, .beta. strand or coil is made by taking the majority among the observations at each residue site. Besides 325 proteins in the structural **library**, 77 proteins were selected from the latest release of the Brookhaven Protein Data Bank, and they were divided into three data sets. Data set 1 was used as a training set for which several adjustable parameters in the method were optimized. Then, the final form of the method was applied to a testing set (data set 2) which contained proteins of chain length .ltoreq.400 residues. The av. prediction accuracy was as high as 69% in the three-state assessment of .alpha., .beta. and coil. Data set 3 contains only those proteins of length >400 residues, for which the present method would not work properly because of the size effect inherent in the 3D-1D compatibility method. The proteins in data set 3 were, therefore, subdivided into constituent domains (data set 4) before being fed into the prediction program. The prediction accuracy for data set 4 was 66% on av., a few percent lower than that for data set 2. Possible causes for this discrepancy are discussed.

L7 ANSWER 29 OF 47 CA COPYRIGHT 2003 ACS on STN
TI Evolutionary similarity among peptide segments is a basis for prediction
of protein folding
AU Sweet, Robert M.
SO Biopolymers (1986), 25(8), 1565-77
CODEN: BIPMAA; ISSN: 0006-3525
PY 1986
AB Short segments of polypeptide, from a protein for which the primary
sequence but not the 3-dimensional structure is known, are compared to a
library of known structures. The basis of comparison is the
probability with which residues in the unknown segment might substitute
through evolution for residues in segments of known structure. In test
cases, segments from known structures that are similar in sequence to
those from a protein treated as unknown are often found to be similar in
3-dimensional structure to one another and to the true structure of the
unknown segment. This provides a basis for prediction of the local
configuration (**secondary** structure) of **polypeptides**.

FILE 'CA, MEDLINE' ENTERED AT 09:33:55 ON 22 SEP 2003

L1	199 S PRIMARY(5W)LIBR?
L2	11 S L1 AND SECONDARY(10W)LIBR?
L3	0 S SECONDARY(6W)SCAFFOLD(4W) (PROTEINS OR POLYPEPTIDES)
L4	2804 S SECONDARY(6W) (PROTEINS OR POLYPEPTIDES)
L5	62 S L4 AND LIBR?
L6	0 S L5 AND PRIMARY(6W)LIBR?(6W) (VARIANT? OR MUTA?)
L7	47 S L5 NOT 2002-2003/PY